

Docusate sodium  
577-11-7 | DTXSID8022959

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 15100 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.41e-01

Confidence level: 5.82e-01

Nearest Neighbors from the Training Set

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Di(2-ethylhexyl) phthalate

Measured: 87100

Predicted: 42800

Image not found

Bis(2-ethylhexyl) terephthalate

Measured: 14500

Predicted: 12500

Image not found

Di(2-ethylhexyl) adipate

Measured: 15500

Predicted: 14400

Image not found

Dioctyl phthalate

Measured: 24000

Predicted: 17100